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* * *	* *	* *	* *	* Welcome to STN International * * * * * * * * * *
NEWS	1			Web Page for STN Seminar Schedule - N. America
NEWS	2	DEC	01	ChemPort single article sales feature unavailable
NEWS	3	APR	03	CAS coverage of exemplified prophetic substances
				enhanced
NEWS		APR		
NEWS	5	APR	24	
				information
NEWS	6	APR	26	USPATFULL and USPAT2 enhanced with patent
	_			assignment/reassignment information
NEWS		APR		CAS patent authority coverage expanded
NEWS		APR		ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS	9	APR	28	Limits doubled for structure searching in CAS
				REGISTRY
NEWS				
				STN on the Web enhanced
NEWS	12	MAY	11	BEILSTEIN substance information now available on
	4.0			STN Easy
NEWS	13	MAY	14	DGENE, PCTGEN and USGENE enhanced with increased
				limits for exact sequence match searches and introduction of free HIT display format
NEWS	2.4	1/2.1/	2.5	INPADOCDB and INPAFAMDB enhanced with Chinese legal
MEMS	14	PIAI	13	status data
NEWS	1.5	MAY	28	
MEMP	10	LIMI	20	records back to 1992
NEWS	16	.TIIN	0.1	CAS REGISTRY Source of Registration (SR) searching
HEND	10	0011	01	enhanced on STN
				cinaneca on our
NEWS	EXP	RESS	MAY	26 09 CURRENT WINDOWS VERSION IS V8.4,
				CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

Enter NEWS followed by the item number or name to see news on that specific topic.

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=> file registry COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.22 0.22

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 10:54:48 ON 17 JUN 2009
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STRUCTURE FILE UPDATES: 15 JUN 2009 HIGHEST RN 1158168-92-3
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 $\label{thm:condition} $$ Uploading C:\Documents and Settings\vrodriguezgarcia\My Documents\e-Red Folder\10586573\Ll.str$

chain nodes:
7 8 9 10 11 13 14 15 16 17
ring nodes:
1 2 3 4 5 6 12 18 19 20 21 22
chain bonds:
6-7 7-8 7-11 8-9 9-10 10-15 11-12 11-13 13-14 13-16 16-17
ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 12-18 12-22 18-19 19-20 20-21 21-22

exact/norm bonds:
7-11 8-9 9-10 10-15 13-14 13-16 16-17
exact bonds:
6-7 7-8 11-12 11-13
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 12-18 12-22 18-19 19-20 20-21 21-22
isolated ring systems:
containing 1 : 12 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom

L1 STRUCTURE UPLOADED

=> s sam sss 11 SAMPLE SEARCH INITIATED 10:55:13 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 29 TO ITERATE

100.0% PROCESSED 29 ITERATIONS 4 ANSWERS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
PROJECTED ITERATIONS: 257 TO 903
PROJECTED ANSWERS: 4 TO 200

L2 4 SEA SSS SAM L1

=> d sca

L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, a-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-ylloxyl-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, sodium salt (1:1)
MF C40 H38 F2 O10 S2. Na

Na

- L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- MF C40 H38 F2 O10 S2
- CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-[[[4,5-bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (\alpha Z)-MF C25 H28 N2 O13 S

- L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[1-[4-(aminosulfonyl)phenyl]-2-(benzoyloxy)ethylidene]-, methyl ester, (Z)- (9CI)$
- MF C24 H21 N O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s full sss l1

100.0% PROCESSED

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END;y FULL SEARCH INITIATED 11:12:39 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 767 TO ITERATE

SEARCH TIME: 00.00.01

84 ANSWERS

L3 84 SEA SSS FUL L1

=> d sca

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

767 ITERATIONS

- IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-
- MF C24 H28 F2 N O6 S
- CI COM

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, (αZ)-MF C25 H30 O7 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, 2-(diethylamino)ethyl ester, (<math>\alpha$ Z)-
- MF C29 H38 N2 O9 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]l-oxo-4-[((2Z)-1-oxo-2-propyloctyl]oxy]-2-buten-1-yl]oxy]-N,N,N-trimethylbromide (1:1)
- MF C33 H46 F2 N O6 S . Br

Absolute stereochemistry. Double bond geometry as shown.

• Br-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 4,5-bis(nitrooxy)pentyl ester,
- (αZ)-MF C24 H26 N2 O12 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (\alpha Z)-MF C25 H29 N O9 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acety)acy)-1-[4-(methy)sulfony])pheny][ethylidene]-4-fluoro-, 3-[4-[1-methyl-1-(nitrosothio)ethyl]-2-oxo-3-oxazolidinyl]propyl ester, (αZ) -
- MF C28 H31 F N2 O9 S2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN L-Aspartic acid, 4-[(2Z)-3-(3,4-difluoropheny1)-4-ethoxy-2-[4-(methylsulfony1)pheny1]-4-oxo-2-buten-1-y1] ester
- MF C23 H23 F2 N O8 S

Absolute stereochemistry.
Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-,
- 3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester
- MF C36 H32 O10 S2
- CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-[[(4-bromobutoxy)carbony1]oxy]-1-[4-(methylsulfony1)pheny1]ethylidene]-, methyl ester, (αZ)-

MF C23 H25 Br 07 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(benzoyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI)
- MF C25 H22 O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
 IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-
- IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)
- MF C24 H29 F N O6 S . Br

• Br-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (22)-2-[4-(methyleuifonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-oxo-3-phenyl-2-buten-1-yl ester
- MF C30 H38 N2 O11 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, a-[1-[4-(methylsulfonyl)phenyl]-2-[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, ethyl ester, (aZ)-
- MF C26 H31 N O10 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-4-[[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)carbonyl)oxy]-3-[4-(mthyloyl-2hydroyl)bhouyl-1-2ng-2-bhts-1-ylloyl-N,N-krimethyl-1-2ng-2-bhts-1-ylloyl-N,N-krimethyl-1-2ng-2-bhts-1-ylloyl-N,N-krimethyl-1-2ng-2-bhts-1-ylloyl-N,N-krimethyl-1-2ng-2-bhts-1-ylloyl-N,N-krimethyl-1-2ng-2-bhts-1-ylloyl-N,N-krimethyl-1-2ng-2-bhts-1-ylloyl-N-krimethyl
- (methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-MF C36 H42 F2 N O8 S

Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (5R)-5,6-bis(nitrooxy)hexyl ester, (α Z)-
- MF C25 H28 N2 O12 S

Absolute stereochemistry. Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α =[2-[[3-(bromomethy1)benzoy1]oxy]-1-[4-(methylsulfony1)phenyl]ethylidene]-, methyl ester, (αZ) -MF C26 H23 Br O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, methyl ester, (α Z)-MF C22 H33 F06 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (aZ)-, (2S)-2-amino-3-ethoxy-3-oxopropyl ester, 2,2,2-trifluoroacetate (1:1) C24 H25 F2 N O8 S . C2 H F3 O2

MF

CM

Absolute stereochemistry. Double bond geometry as shown.

CM 2

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[2-[[4-(acetyloxy)-2-(3-fluoropheny1)-4-methyl-3-[4-(methylsulfony1)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]proylidene]-3-fluoro-, sodium salt (1:1)$
- MF C40 H38 F2 O10 S2 . Na

Na

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid, $\alpha = [2-[3-[[(1,1-\dim thy)]]] - [4-(\min thy)]]$ methylbulfonyl)phenyl]ethylidene]-, methyl ester, $(\alpha 2)$ -MF C32 H38 07 S Si

^{**}PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-,
- (2S)-2-amino-3-ethoxy-3-oxopropyl ester
 MF C24 H25 F2 N O8 S

Absolute stereochemistry.

Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-,
 (22)-4-[(6-bromohexyl)oxy]-2-[4-(methylsulfonyl)phenyl]-4-oxo-3-phenyl-2buten-1-yl ester
- MF C30 H38 Br N O8 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[6-
- (nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, (aZ)-
- MF C25 H29 N O10 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 1H-Benzimidazole-4-carboxylic acid,

2-ethoxy-1-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl)methyl]-, (22)-3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-vl ester

MF C43 H36 F2 N6 O7 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5,6-bis(nitrooxy)hexyl ester, (αZ)-
- MF C25 H28 N2 O12 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 1.3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[3-[[[(1,1dimethylethyl)dimethylsilyl]oxy]methyl]benzoyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αΕ)-C32 H38 O7 S Si

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-IN
- (aminosulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI) MF C19 H18 F N O6 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (2S)-2-amino-3-ethoxy-3-oxopropyl ester, (αZ)MF C24 H25 F2 N O8 S
- CI COM

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester, sodium salt (1:1)
- MF C36 H32 O10 S2 . Na

Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

 10 Benzeneacetic acid, ac=[1-[4-(methylsulfonyl)]phenyl]-2-[[[3[(nitrooxy)methyl]phenoxy]carbonyl]oxy]ethylidene]-, methyl ester,
 (aZ)-
- MF C26 H23 N O10 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzenepropanoic acid, β -[(1-oxopropoxy)methyl]- α -phenyl-, ethyl ester
- MF C21 H24 O4

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)

MF C24 H28 F2 N O6 S . Br

● Br-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, 6-bromohexyl ester, (α Z)-MF C25 H29 Br O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[1-[4-(methylsulfonyl)phenyl]-2-[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, ethyl ester, (α Z)-

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 1H-Benzimidazole-7-carboxylic acid, 2-ethoxy-1-[[2'-(2H-etrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, 3-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1oxo-2-buten-1-yl]oxy]-2-oxopropyl ester
- MF C46 H39 F N6 O10 S

PAGE 1-A

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, phenylmethyl ester, (α Z)-
- MF C28 H26 N2 O13 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[2-[[[3-(bromomethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, <math>(\alpha Z)$ -
- MF C26 H23 Br 07 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- TN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-
- (aminosulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) MF C19 H17 F2 N 06 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN L3
- Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-IN (methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N, N, N-trimethyl-MF C24 H29 F N O6 S
- COM

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneactic acid, a-[2-[[4-(acetyloxy)-2-(3,4-difluoropheny1)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-
- MF C36 H28 F4 O10 S2
- CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, 2-(diethylamino)ethyl$

ester, hydrochloride (1:1), (αZ)-C29 H38 N2 O10 S . C1 H

Double bond geometry as shown.

ME

HC1

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha [2-[4-[(22)-4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-1-oxobutoxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, <math>(\alpha Z)$ -
- MF C44 H44 F2 O12 S2
- CI COM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- (methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester (9CI) MF C25 H30 F2 N2 O6 S

Absolute stereochemistry. Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4oxo-3-phenyl-2-buten-1-yl ester
- MF C25 H30 N2 09 S
- CI COM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid, $\alpha - [1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-(methylsulfonyl)phenyl]]$

1-oxohexyl]oxy]ethylidene]-, methyl ester, (αZ) -

F C24 H27 N O9 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, ~[2-(acetyloxy)-1-[4(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-,
(2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-ethoxy-3-oxopropyl ester,
(dZ)
MF C29 H33 F2 N 010 S

Absolute stereochemistry. Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (α Z)-
- MF C23 H24 N2 O13 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[[3-(hydroxymethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (α Z)-
- MF C26 H24 08 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[1-[4-(aminosulfony1)pheny1]-2-(benzoyloxy)ethylidene]-, methyl ester, (Z)- (9CI)$
- MF C24 H21 N 06 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-final content of the conte
- MF CZ4 HZ8 FZ N OE CI COM

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, 3-(3,4-difluorophenyl)-4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-[4-(methylsulfonyl)phenyl]-2-buten-1-yl ester C42 H44 F4 O9 S2 Si
- MF

$$\begin{array}{c} \text{Ne} \\ \text{t-Bu-Si-O} \\ \text{CH}_2 \\ \text{C-CH}_2 \\ \text{O-C-C-C-C} \\ \text{C-R} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α -[1-[4-(methylsulfonyl)phenyl]-2-[[[[5-

(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, (α Z)-MF C24 H27 N O10 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN INDEX NAME NOT YET ASSIGNED MF C44 H44 F2 O12 S2 . Na

Double bond geometry as shown.

Na

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α-[2-[(2S)-2-amino-3-hydroxy-1-oxopropoxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester (9CI) MF C22 H23 F2 N O7 S

Absolute stereochemistry. Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, 7-(nitrooxy)heptyl ester, (α Z)-MF C26 H31 N O9 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α -[1-[4-(methylsulfonyl)phenyl]-2-[[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, methyl ester, (α Z)-

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Ethanaminium, 2-||(2Z)-4-(acetyloxy)-2-(3-fluoro
- IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)
- MF C24 H29 F N O6 S . Br

Double bond geometry as shown.

● Br-

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha [2-[[[[4,5-$

bis(nitrooxy)pentyl]oxy|carbonyl]oxy]-1-[4- (methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (\alpha Z)- MF C25 H28 N2 013 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

Benzeneacetic acid, α-[2-[[3-[[(1,1dimethylathyl)dimethylsilyl]oxy]methyl]phenoxy]carbonyl]oxy]-1-[4(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)
MF C32 H38 08 S Si

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
- (aminosulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI) MF C19 H19 N O6 S

Double bond geometry as shown.

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT **

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α =[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 1,6-hexanediyl ester, (α Z, α 'Z)- (9CI)
- MF C44 H46 O12 S2

Double bond geometry as shown.

$$\begin{array}{c} \text{Ne} & \text{Ph} & \text{Ph} \\ \text{Z} & \text{O} & \text{(CH2)6} \\ \text{AcO} & \text{OAc} \\ \end{array}$$

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha=[2-[[4-(acetyloxy]-2-(3,4-difluoropheny1)-3-[4-(methylsulfony1)pheny1]-1-oxo-2-buten-1-y1]oxy]-1-[4-(methylsulfony1)pheny1]ethylidene]-3,4-difluoro-, sodium salt (1:1)$
- MF C36 H28 F4 O10 S2 . Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha = [1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-$
- 1-oxohexyl]oxy]ethylidene]-, (1S)-1-carboxyethyl ester, (α Z)-MF C26 H29 N O11 S

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

TN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-4-[[(2R)-1-oxo-2-propylocty1]oxy]-2-buten-1-y1]oxy]-N,N,N-trimethy1-

C33 H46 F2 N O6 S ME

COM

Absolute stereochemistry.

Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN L-Aspartic acid, 4-[3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-yl] ester
- MF C23 H23 F2 N O8 S

Absolute stereochemistry. Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-

(methylsulfony1)phenyl]ethylidene]-, 5-(nitrooxy)pentyl ester, (αZ)-MF C24 H27 N O9 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[1-[4-(methylsulfonyl)phenyl]-2-[[3-
- [(nitrooxy)methyl]benzoyl]oxy]ethylidene]-, methyl ester, (αZ)-MF C26 H23 N O9 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1.1)
- MF C24 H28 F2 N O6 S . Br

Double bond geometry as shown.

• Br-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[[[4,5-bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)penyl]ethylidene]-, methyl ester, (α Z)-MF C24 H26 N2 013 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α -[2-[[[(6-bromohexyl)oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (α Z)-

MF C26 H31 Br 07 S

Double bond geometry as shown.

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT **

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI)
 MF C20 H19 F O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

$$\begin{array}{c|c} \text{Me-} \\ \text{S} \\ \text{O} \\ \text{C} \\ \text{C}$$

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[1-[4-(methylsulfonyl)phenyl]-2-[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, 2-(diethylamino)ethylester, (αZ) -
- MF C29 H38 N2 O10 S
- CI COM

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-2-(1,1-dimethylethoxy)-1-methyl-2-oxoethyl ester, (αZ)-
- MF C30 H37 N O11 S

Absolute stereochemistry. Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, 3,4-difluoro- α -[1-[4-(methylsulfonyl)phenyl]-2-[(2R)-1-oxo-2-propyloctyl]oxy]ethylidene]-, methyl ester, (α Z)-MF C29 H36 F2 O6 S

Absolute stereochemistry.
Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3,4-bis(nitrooxy)butyl ester, <math>(\alpha\mathbb{Z})-$
- MF C23 H24 N2 O12 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-
- oxo-3-phenyl-2-butenyl ester, monohydrochloride (9CI) MF C25 H30 N2 O9 S . Cl H

Double bond geometry as shown.

HC1

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, \(\alpha\) - \((2 - (\acety\)) - 1 - [4 - (\amplitum \) \) (\amplitum \) (\amplitum

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[(2S)-2,6-diamino-1-oxohexyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester, (αE) (9CI)
- MF C25 H30 F2 N2 O6 S

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha = [2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl$

 $3-[4-(\mathsf{methylsulfonyl})\mathsf{phenyl}]-1-\mathsf{oxo}-2-\mathsf{penten}-1-yl]\mathsf{oxy}]-2-\mathsf{methyl}-1-[4-(\mathsf{methylsulfonyl})\mathsf{phenyl}]\mathsf{propylidene}]-3-fluoro-$

MF C40 H38 F2 O10 S2

COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

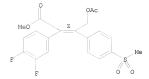
- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[(4-bromobutoxy)carbonyl]oxy]-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (αZ)-MF C24 H27 Br O7 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) MF C20 H18 F2 O6 S



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SINCE FILE TOTAL ENTRY SESSION 201.24 201.46

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ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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E2 2 US2006-586567/AP

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1 --> US2006-586573/AP
E4
            0 US2006-586573/PRN
E5
                  US2006-586574/AP
            1
E6
                 US2006-586575/AP
US2006-586576/AP
            1
E7
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E8
            1
                 US2006-586577/AP
                 US2006-586578/AP
E9
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            1 US2006-586579/AP
1 US2006-586581/AP
E10
E11
E12
                 US2006-586583/AP
=> s us2006-586573/apps
             1 US2006-586573/AP
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0 US2006-586573/PRN 1.4 1 US2006-586573/APPS (US2006-586573/AP,PRN)

=> sel rn E1 THROUGH E34 ASSIGNED

=> file registry COST IN U.S. DOLLARS

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http://www.cas.org/support/stngen/stndoc/properties.html

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                  (10102-43-9/RN)
              1 108-24-7/BI
                  (108-24-7/RN)
              1 122-04-3/BI
                  (122-04-3/RN)
             1 14739-12-9/BI
                  (14739-12-9/RN)
             1 14739-15-2/BI
                  (14739-15-2/RN)
             1 14739-16-3/BI
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(14739-16-3/RN)

1 14739-18-5/BI (14739-18-5/RN)

1 14739-19-6/BI

(14739-19-6/RN)

1 162011-90-7/BI (162011-90-7/RN)

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(179174-76-6/RN)

1 179174-77-7/BI

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1 18343-90-3/BI

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1 861655-84-7/BI

(861655-84-7/RN)

1 861655-85-8/BI (861655-85-8/RN)

(861655-85-87RI

1 861655-86-9/BI

(861655-86-9/RN)

34 (10102-43-9/BI OR 108-24-7/BI OR 122-04-3/BI OR 14739-12-9/BI OR 14739-15-2/BI OR 14739-15-6/BI OR 14739-15-6/BI OR 1739-13-6-6/BI OR 1739-13-6-6/BI OR 162011-90-7/BI OR 179174-76-6/BI OR 179174-77-7/BI OR 179174-79-9/BI OR 18343-90-3/BI OR 3068-00-6/BI OR 329900-75-6/B I OR 329967-85-3/BI OR 50-78-2/BI OR 5048-26-0/BI OR 573-34-7/B

I OR 654068-92-5/BI OR 6835-50-3/BI OR 754242-03-0/BI OR 77-76-9 /BI OR 7761-88-8/BI OR 821-41-0/BI OR 849139-06-6/BI OR 861405-2 6-7/BI OR 861405-28-9/BI OR 861405-33-6/BI OR 861405-34-7/BI OR 861655-83-6/BI OR 861655-84-7/BI OR 861655-85-8/BI OR 861655-86-9/BI)

=> s 13 and 15 L6 4 L3 AND L5

=> d sca

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 4,5-bis(nitrooxy)pentyl ester, (αZ) -

MF C24 H26 N2 O12 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3,4-bis(nitrooxy)butyl ester, (α 2)-
- MF C23 H24 N2 O12 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5,6-bis(nitrooxy)hexyl ester, (αZ)-

MF C25 H28 N2 O12 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (5R)-5,6-bis(nitrooxy)hexyl ester, (<math>\alpha Z$)-
- MF C25 H28 N2 O12 S

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

2.40

209.76

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=> s 13

=> s 17 and (nitrosated or nitrosylated)

604 NITROSYLATED

1 L7 AND (NITROSATED OR NITROSYLATED)

=> d sca

L8

L8 1 ANSWERS ZCAPLUS COPYRIGHT 2009 ACS on STN

IC ICM A61K031-40

ICS A61K031-415; A61K031-421; A61K031-50; C07D207-325; C07D231-06; C07D237-14; C07D263-04; C07D263-06

CC 21-2 (General Organic Chemistry)

Section cross-reference(s): 1

II Preparation of nitrosated and nitrosylated

```
cyclooxygenase-2 inhibitors
cyclooxygenase 2 inhibitor nitrosated nitrosylated
prepn
Analgesics
Anti-inflammatory agents
   (preparation of nitrosated and nitrosylated
   cyclooxygenase-2 inhibitors)
Nitroso compounds
Nitrosvl complexes
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
   (preparation of nitrosated and nitrosylated
   cvclooxygenase-2 inhibitors)
329900-75-6, cyclooxygenase-2
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
(Biological study); PROC (Process)
   (mediated disorders; treatment; preparation of nitrosated and
   nitrosylated cyclooxygenase-2 inhibitors)
205580-05-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)
   (preparation of nitrosated and nitrosylated
   cyclooxygenase-2 inhibitors)
                           346683-71-4P 346683-72-5P
346683-69-0P 346683-70-3P
                                                           346683-73-6P
              346683-76-9P
                             346683-77-0P
                                            346683-78-1P
                                                          346683-79-2P
346683-75-8P
346683-80-5P 346683-81-6P 346683-82-7P 346683-83-8P
346683-84-9P
              346683-85-0P 346683-86-1P 346683-87-2P 346683-88-3P
347162-90-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
   (preparation of nitrosated and nitrosylated
   cvclooxvgenase-2 inhibitors)
346683-99-6P
              346684-20-6P
                            346684-22-8P
RL: BYP (Byproduct); PREP (Preparation)
   (preparation of nitrosated and nitrosylated
   cvclooxygenase-2 inhibitors)
52-67-5, D-Penicillamine
                         53-86-1, Indomethacin
                                                  78-83-1.
2-Methyl-1-propanol, reactions 78-94-4, Methyl vinyl ketone, reactions
100-53-8, Benzyl mercaptan 627-18-9, 3-Bromo-1-propanol 1445-73-4,
1-Methyl-4-piperidone 1778-09-2, 4-Methylthioacetophenone 2417-72-3,
Methyl 4-bromomethylbenzoate
                             3446-89-7, 4-Methylthiobenzaldehyde
18162-48-6, tert-Butyldimethylsilyl chloride 21382-98-9,
4-Methylthiobenzonitrile 24214-73-1, Cyclohexylhydrazine hydrochloride
32047-53-3, 1-Amino-2-methyl-2-propanethiol hydrochloride 61040-78-6,
                               90878-19-6. Phenethylmagnesium chloride
2.4.6-Trimethoxybenzyl alcohol
194596-99-1
RL: RCT (Reactant); RACT (Reactant or reagent)
   (preparation of nitrosated and nitrosylated
   cvclooxygenase-2 inhibitors)
15581-80-3P
             28399-82-8P
                          40027-88-1P
                                         73303-88-5P.
2-Methyl-2-mercapto-1-propanol 86864-60-0P
                                             89031-84-5P
                                                           136881-95-3P
157672-00-9P
              170571-19-4P 170571-20-7P
                                            170571-71-8P
                                                          179174-91-5P
179174-92-6P
               179174-93-7P
                            179174-94-8P
                                            181695-72-7P
                                                          181695-81-8P
213764-17-1P
                                                          346683-90-7P
346683 - 91 - 8P 346683 - 92 - 9P 346683 - 94 - 1P 346683 - 95 - 2P 346683 - 96 - 3P
346683-97-4P 346683-98-5P 346684-00-2P 346684-01-3P 346684-02-4P
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346684-03-5P 346684-04-6P 346684-05-7P 346684-06-8P 346684-07-9P

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346684-08-0P 346684-09-1P 346684-10-4P 346684-11-5P 346684-12-6P
     346684-13-7P 346684-14-8P 346684-15-9P 346684-16-0P 346684-18-2P 346684-19-3P 346684-21-7P 347162-91-8P
                                                                346684-17-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of nitrosated and nitrosylated
        cyclooxygenase-2 inhibitors)
     346684-23-9P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of nitrosated and nitrosylated
        cyclooxygenase-2 inhibitors)
ALL ANSWERS HAVE BEEN SCANNED
=> s 17 and (nitrosated or nitrosylated or NO or (nitric (w) oxide))
          1340 NITROSATED
          604 NITROSYLATED
       3932570 NO
        220094 NOS
          2032 NOES
       4060112 NO
                 (NO OR NOS OR NOES)
        223122 NITRIC
             3 NITRICS
        223125 NITRIC
                 (NITRIC OR NITRICS)
       1991269 OXIDE
       377613 OXIDES
       2097881 OXIDE
                 (OXIDE OR OXIDES)
        131578 NITRIC (W) OXIDE
            11 L7 AND (NITROSATED OR NITROSYLATED OR NO OR (NITRIC (W) OXIDE))
=> d sca
     11 ANSWERS ZCAPLUS COPYRIGHT 2009 ACS on STN
     ICM C07C317-24
     ICS A61K031-21
INCL 514509000; 558482000
    25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
     Section cross-reference(s): 1
    Process for making nitric oxide releasing prodrugs of
    diary1-2-(5H)-furanones as cyclooxygenase-2 inhibitors
    nitric oxide releasing prodrug diphenylbutenoate hexyl
    nitrate
     Drug delivery systems
        (prodrugs; preparation of nitric oxide releasing
        prodrugs of diarv1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     329900-75-6, Cyclooxygenase 2
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (inhibitors; preparation of nitric oxide releasing
        prodrugs of diarv1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     10102-43-9, Nitric oxide, biological studies
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (preparation of nitric oxide releasing prodrugs of
        diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     64-19-7, Acetic acid, uses 67-68-5, Dmso, uses 68-12-2, Dmf, uses
     75-05-8, Acetonitrile, uses 75-09-2, Dichloromethane, uses 75-52-5,
     Nitromethane, uses 127-19-5, N,N-Dimethylacetamide
                                                           872-50-4,
     1-Methyl-2-pyrrolidinone, uses 1300-21-6, Dichloroethane 25321-22-6,
     Dichlorobenzene
```

1.9

L9

ΤТ

```
(preparation of nitric oxide releasing prodrugs of
        diary1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     937-14-4, m-Chloroperbenzoic acid 1504-58-1, 3-Phenyl-2-propyn-1-ol
     4286-55-9 7722-84-1, Hydrogen peroxide, reactions 10058-23-8,
     Potassium peroxymonosulfate
                                 11138-47-9, Sodium perborate
                                                                  74087-85-7,
                       78948-87-5, Magnesium monoperoxyphthalate
     Dimethyldioxirane
     210292-04-9, 4-Methylthiophenylmagnesium chloride
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of nitric oxide releasing prodrugs of
        diary1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     176594-44-8P
                   179174-79-9P 754242-10-9P 754242-11-0P
     754242-12-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of nitric oxide releasing prodrugs of
        diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     754241-98-0P
     RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
        (preparation of nitric oxide releasing prodrugs of
        diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0
=> d ibib hitstr 1-11
THE ESTIMATED COST FOR THIS REQUEST IS 42.79 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N:v
   ANSWER 1 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:
                        2008:465556 ZCAPLUS
DOCUMENT NUMBER:
                         148:523285
TITLE:
                         Development of a discriminating in vitro dissolution
                        method for a poorly soluble NO-donating
                         selective cyclooxygenase-2 inhibitor
AUTHOR(S):
                         Papp, Robert; Luk, Pauline; Mullett, Wayne M.; Kwong,
                         Elizabeth; Debnath, Smita; Thibert, Roch
CORPORATE SOURCE:
                         Drug Metabolism and Pharmacokinetics, Merck Frosst
                        Center for Therapeutic Research, Kirkland, QC, H9H
                        3L1, Can.
SOURCE:
                        Journal of Pharmaceutical and Biomedical Analysis
                        (2008), 47(1), 16-22
                        CODEN: JPBADA; ISSN: 0731-7085
PUBLISHER:
                        Elsevier B.V.
DOCUMENT TYPE:
                        Journal
LANGUAGE:
                        English
     754241-98-0
     RL: PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (development of discriminating in vitro dissoln, method for poorly soluble
        NO-donating cyclooxygenase-2 inhibitor)
     754241-98-0 ZCAPLUS
RN
CN
     Benzeneacetic acid, a-[2-(acetyloxy)-1-[4-
     (methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (\alpha Z)-
     (CA INDEX NAME)
```

RL: NUU (Other use, unclassified); USES (Uses)

REFERENCE COUNT:

18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN 2006:495882 ZCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

145:14695

TITLE: Compounds for targeting mechanisms implicated in the

progression of stroke INVENTOR(S):

Munoz, Benito; Pavne, Joseph E.; Prasit, Petpiboon; Reger, Thomas S.; Smith, Nicholas D.; Stock, Nicholas

S.; McGuire, Angela R. Merck & Co., Inc., USA PATENT ASSIGNEE(S): PCT Int. Appl., 63 pp. SOURCE:

CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

KIND PATENT NO. DATE APPLICATION NO. DATE WO 2006055404 A2 20060526 WO 2005-US40851 20051110 WO 2006055404 A3 20060810 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN. YU. ZA. ZM. ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM PRIORITY APPLN. INFO.: US 2004-628280P P 20041116 OTHER SOURCE(S): MARPAT 145:14695

887908-51-2P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(compds. for targeting mechanisms implicated in progression of stroke) 887908-51-2 ZCAPLUS

1H-Benzimidazole-7-carboxylic acid,

2-ethoxy-1-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, 3-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1oxo-2-buten-1-y1]oxy]-2-oxopropy1 ester (CA INDEX NAME)

PAGE 1-B

IT 887908-54-5 887908-56-7
RI: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (compds. for targeting mechanisms implicated in progression of stroke)

RN 887908-54-5 ZCAPLUS

CN 1H-Benzimidazole-4-carboxylic acid,
2-ethoxy-1-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-,
(22)-3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2buten-1-yl ester (CA INDEX NAME)

RN 887908-56-7 ZCAPLUS

CN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-4-[[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)carbonyl]oxy]-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N, N, N-trimethyl- (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT:

1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 2006:383478 ZCAPLUS

DOCUMENT NUMBER: 144:432558

TITLE: Preparation of methylsulfonylphenylalkenoates as water soluble prodrugs of COX-2 inhibitors.

INVENTOR(S): Munoz, Benito; Payne, Joseph Edward; Prasit,

Petpiboon; Reger, Thomas S.; Smith, Nicholas D.; Stock, Nicholas S.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA SOURCE: PCT Int. Appl., 60 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patient. LANGUAGE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

DATEME	NO			ETNI		Da TE			2 DDI	TORT	TON	NIO.		D	a mrz			
PAIENI	PATENT NO.					KIND DATE					APPLICATION NO.							
NO 2006	WO 2006044230					2006	0427					20051007						
W0 2000				AM, AT, AU, AZ,														
w:																		
									DZ,									
									IS,									
									MA,									
									PL,									
					TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,		
			ZM,															
RW:	ΑT,																	
									PΤ,									
									ML,									
							SD,	SL,	SZ,	ΤZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,		
			MD,	RU,	ΤJ,	TM												
IORITY APP									US 2	004-	6179	62P		P 2	0041	012		
HER SOURCE	(S):			MARI	PAT	144:	4325	58										
885020-	33-7	P 88	5020	-34-	8P 8	8502	0-36	-0P										
885020-	37-1	P 88	5020	-38-	2P													
RL: PAC	(Ph	arma	colo	gica.	l ac	tivi	ty);	SPN	(Sy	nthe	tic ;	prep	arat	ion)	; TH	U		
(Therap	euti	c us	e); 1	BIOL	(Bi	olog	ical	stu	dy);	PRE	P (P	repa:	rati	on);	USE	S		
(Uses)						-												
(cla	imed	com	poun	d; p	repa	rati	on o	f me	thy1:	sulf	onyl	phen	ylal	keno	ates	as '		

soluble prodrugs of COX-2 inhibitors)

885020-33-7 ZCAPLUS RN

CN Ethanaminium, 2-[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N, N, N-trimethyl- (CA INDEX NAME)

Double bond geometry as shown.

RN 885020-34-8 ZCAPLUS

CN Ethanaminium, 2-[[(2Z)-4-(acetvloxv)-2-(3-fluorophenv1)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl- (CA INDEX NAME)

RN 885020-36-0 ZCAPLUS

CN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3, 4-difluoro-, (αZ) -, (2S)-2-amino-3-ethoxy-3-oxopropyl ester, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 885020-35-9 CMF C24 H25 F2 N O8 S

Absolute stereochemistry. Double bond geometry as shown.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 885020-37-1 ZCAPLUS

CN L-Aspartic acid, 4-[(2Z)-3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-yl] ester (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

- RN 885020-38-2 ZCAPLUS
- CN Benzeneacetic acid, α-[2-[[(2S)-2,6-diamino-1-oxohexyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester, (κΕ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

IT 885020-42-8P 885020-43-9P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of methylsulfonylphenylalkenoates as water soluble prodrugs of COX-2 inhibitors)

- RN 885020-42-8 ZCAPLUS
- CN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)penyl)-1-oxo-2-buten-1-yl]oxy]-N, N, N-trimethyl-, bromide (1:1) (CA INDEX NAME)

Br -

RN 885020-43-9 ZCAPLUS

CN Ethanaminium, 2-[[(22)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N, N, N-trimethyl-, bromide (1:1) (CA INDEX NAME)

Double bond geometry as shown.

• Br-

IT 885020-47-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of methylsulfonylphenylalkenoates as water soluble prodrugs of COX-2 inhibitors)

RN 885020-47-3 ZCAPLUS

CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-,

(2S) = $2-[[(1,1-dimethylethoxy)carbonyl]amino] = 3-ethoxy = 3-oxopropyl ester, <math>(\alpha Z)$ = (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1315893 ZCAPLUS

DOCUMENT NUMBER: 144:212486

TITLE: Synthesis of a NO-Releasing Prodrug of Rofecoxib

AUTHOR(S):

Engelhardt, F. Conrad; Shi, Yao-Jun; Cowden, Cameron J.; Conlon, David A.; Pipik, Brenda; Zhou, George;

McNamara, James M.; Dolling, Ulf-H.

CORPORATE SOURCE: Department of Process Research, Merck Company, Rahway,

NJ, 07065-0900, USA

SOURCE: Journal of Organic Chemistry (2006), 71(2), 480-491

CODEN: JOCEAH; ISSN: 0022-3263 PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:212486

ΙT 875783-67-8P

RL: BYP (Byproduct); PREP (Preparation)

(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-pheny1-2-propyn-1-ol)

RN 875783-67-8 ZCAPLUS

CN Benzeneacetic acid, $\alpha - [2-(acetyloxy)-1-[4-$

(methylsulfonyl)phenyl]ethylidene]-, 1,6-hexanediyl ester,

(αZ,α'Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

754242-04-1P

RL: BYP (Byproduct); SPN (Synthetic preparation); PREP (Preparation) (synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-pheny1-2-propyn-1-ol)

754242-04-1 ZCAPLUS RN

CN Benzeneacetic acid, $\alpha = [2-(acetyloxy)-1-[4-$ (methylsulfonyl)phenyl]ethylidene]-, 6-bromohexyl ester, (α Z)- (CA INDEX NAME)

Double bond geometry as shown.

IT 754242-12-1P

CN

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenv1-2-propvn-1-ol)

RN 754242-12-1 ZCAPLUS

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, (α Z)-(CA INDEX NAME)

Double bond geometry as shown.

IT 754241-98-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)

RN 754241-98-0 ZCAPLUS CN Benzeneacetic acid.

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (αZ) -(CA INDEX NAME)

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

14

L9 ANSWER 5 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:963804 ZCAPLUS

DOCUMENT NUMBER: 143:266677

TITLE: Process for making nitric oxide

releasing prodrugs of diary1-2-(5H)-furanones as cvclooxygenase-2 inhibitors

INVENTOR(S): Shi, Yao-Jun; Engelhardt, F. Conrad; Cowden, Cameron

THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS

John; Conlon, David A.; Pipik, Brenda

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 16 pp.

CODEN: USXXCO DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

REFERENCE COUNT:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
US 20050192346	A1	20050901	US 2005-66676	20050225		
PRIORITY APPLN. INFO.:			US 2004-549126P P	20040301		
OTHER SOURCE(S):	CASRE	EACT 143:266	677; MARPAT 143:266677			
IT 754242-12-1P						
RL: RCT (Reactant);	SPN	(Synthetic pr	reparation); PREP (Prepar	ation); RAC		
(Reactant or reagen	t)					
(preparation of	nitrio	c oxide relea	asing prodrugs of			
diary1-2-(5H)-fu	ranone	es as cycloo:	xygenase-2 inhibitors)			
RN 754242-12-1 ZCAPLU	S	-				

RN 754242-12-1 ZCAPLUS CN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, (αZ)-(CA INDEX NAME)

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)

RN 754241-98-0 ZCAPLUS

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-CN

(methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (aZ)-(CA INDEX NAME)

Double bond geometry as shown.

ANSWER 6 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 2005:696873 ZCAPLUS

DOCUMENT NUMBER: 143:172624

TITLE: Preparation of nitric oxide releasing prodrugs of diary1-2(5H)-furanones as

cyclooxygenase-2 inhibitors

Dufresne, Claude; Berthelette, Carl; Li, Lianhai; INVENTOR(S): Guay, Daniel; Gallant, Michel; Lacombe, Patrick;

Aspiotis, Renee; Wang, Zhaovin; Sturino, Claudio F. PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.

SOURCE: PCT Int. Appl., 38 pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.							DATE				ICAT	DATE					
WO 2005070883																	
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO.	CR,	CU,	CZ,	DE,	DK.	DM,	DZ,	EC,	EE,	EG,	ES.	FI,	GB,	GD,
		GE,	GH,	GM,	HR.	HU,	ID,	IL.	IN.	IS,	JP,	KE.	KG,	KP,	KR.	KZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO.	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		TJ,	TM.	TN.	TR.	TT.	TZ,	UA.	UG,	US,	UZ,	VC.	VN.	YU.	ZA.	ZM,	ZW
	RW:						MW,										
		AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,
		MR,	NE,	SN,	TD,	TG											
AU	2005	2062	28		A1		2005	0804		AU 2	005-	2062	28		2	0050	125
CA	2554	334			A1		2005	0804		CA 2	005-	2554	334		2	0050	125
EP	1711	459			A1		2006	1018		EP 2	005-	7064	13		2	0050	125
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	SI,	LT,	LV,	FI,	RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK,	IS	
CN	1914	169			A		2007	0214		CN 2	005-	8000	3263		2	0050	125
JP	2007	5204	83		T		2007	0726		JP 2	006-		20050125				

US 20080242643 A1 20081002 US 2006-586381 20060718 IN 2006DN04347 20070713 IN 2006-DN4347 20060727 A PRIORITY APPLN. INFO.: US 2004-539666P P 20040127 WO 2005-CA83 W 20050125

CASREACT 143:172624; MARPAT 143:172624 OTHER SOURCE(S):

861430-33-3P 861430-34-4P 861430-36-6P

861430-38-8P

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of nitric oxide releasing prodrugs of

diary1-2(5H)-furanones as cyclooxygenase-2 inhibitors)

RN 861430-33-3 ZCAPLUS

CN Benzeneacetic acid, α -[2-[[[[4,5-

bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (aZ)- (CA INDEX NAME)

Double bond geometry as shown.

RN 861430-34-4 ZCAPLUS

CN Benzeneacetic acid, α -[2-[[[4,5bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (aZ)- (CA INDEX NAME)

- RN 861430-36-6 ZCAPLUS
- CN Benzeneacetic acid, $\alpha=[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, <math>(\alpha Z)$ (CA INDEX NAME)

Double bond geometry as shown.

- RN 861430-38-8 ZCAPLUS
- CN Benzeneacetic acid, α -[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, phenylmethyl ester, (α Z)-(CA INDEX NAME)

REFERENCE COUNT: THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 7 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

2005:696865 ZCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 143:193802

TITLE: Preparation of nitric oxide

releasing prodrugs of diary1-2(5H)-furanones as cyclooxygenase-2 inhibitors

INVENTOR(S):

Berthelette, Carl; Li, Lianhai; Beaulieu, Christian; Wang, Zhaoyin; Sturino, Claudio F.

Merck Frosst Canada & Co., Can. PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 41 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PAT	PATENT NO.					KIND DATE					ICAT	DATE					
WO	2005	0708	74		A1 2005080								20050125				
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											EC,						
											JP,						
											SC.						
											UZ,						
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
											BE,						
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							BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,
114	2005				TD,		2005	0804		211 2	2005-	2062	29		2	0.050	125
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											2005-						
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
											CZ,						
	1914										2005-						
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	2008										2006-						
PRIORITY					n		2007	0,13			2004-					0040	

OTHER SOURCE(S): CASREACT 143:193802; MARPAT 143:193802

IT 861655-83-6P 861655-84-7P 861655-85-8P

861655-86-9P

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL

(Biological study); PREP (Preparation); USES (Uses)
(preparation of nitric oxide releasing prodrugs of

diaryl-2(5H)-furanones as cyclooxygenase-2 inhibitors)

RN 861655-83-6 ZCAPLUS

CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5,6-bis(nitrooxy)hexyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

RN 861655-84-7 ZCAPLUS

CN Benzeneacetic acid, a-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (5R)-5,6-bis(nitrooxy)hexyl ester, (aZ)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 861655-85-8 ZCAPLUS

CN Benzeneacetic acid, a-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 4,5-bis(nitrooxy)pentyl ester, (aZ)- (CA INDEX NAME)

861655-86-9 ZCAPLUS RN

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3,4-bis(nitrooxy)butyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT: THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 8 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:739958 ZCAPLUS DOCUMENT NUMBER: 141:260542

TITLE: Preparation of nitric oxide

releasing prodrugs of diary1-2-(5H)-furanones as

selective cvclooxvgenase-2 inhibitors

INVENTOR(S): Berthelette, Carl; Li, Lianhai; Sturino, Claudio;

Wang, Zhaoyin

PATENT ASSIGNEE(S): Merck Frosst Company, Can. SOURCE:

U.S. Pat. Appl. Publ., 19 pp.

CODEN: USXXCO Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

DOCUMENT TYPE:

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		-												
US 2004017633	31	A1	2	20040	0909	1	US 2	004-	7902	88		2	0040	301
US 7169809		B2	2	2007	0130									
AU 2004240700	AU 2004240700 A1						AU 2	004-2	20040301					
CA 2517490	CA 2517490 A1					(CA 2	004-2	20040301					
WO 2004103955	WO 2004103955				1202	02 WO 2004-CA314						20040301		
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NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
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             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
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             TD, TG
     EP 1601644
                          A1
                                20051207
                                            EP 2004-761562
                                                                    20040301
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                          В1
                                20090527
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK
     JP 2007516954
                          Т
                                20070628
                                            JP 2006-529472
                                                                    20040301
PRIORITY APPLN. INFO.:
                                            US 2003-452124P
                                                                   20030305
                                            WO 2004-CA314
                                                                 W 20040301
OTHER SOURCE(S):
                         MARPAT 141:260542
    754241-98-0P 754241-99-1P 754242-00-7P
     754242-01-8P 754242-02-9P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of nitric oxide releasing prodrugs of
        diarylfuranones as selective COX-2 inhibitors)
     754241-98-0 ZCAPLUS
RN
CN
     Benzeneacetic acid, a-[2-(acetyloxy)-1-[4-
     (methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (\alphaZ)-
     (CA INDEX NAME)
```

RN 754241-99-1 ZCAPLUS

CN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4oxo-3-phenyl-2-butenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 754242-00-7 ZCAPLUS

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5-(nitrooxy)pentyl ester, (α Z)-(CA INDEX NAME)

Double bond geometry as shown.

RN 754242-01-8 ZCAPLUS

CN Benzeneacetic acid, α =[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 7-(nitrooxy)heptyl ester, (α Z)-(CA INDEX NAME)

Double bond geometry as shown.

RN 754242-02-9 ZCAPLUS

CN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4oxo-3-phenyl-2-buten-1-yl ester (CA INDEX NAME)

IT 754242-04-1P 754242-08-5P 754242-09-6P

754242-12-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)

RN 754242-04-1 ZCAPLUS

CN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 6-bromohexyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

RN 754242-08-5 ZCAPLUS

CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (22)-4-[(6-bromohexyl)oxy]-2-[4-(methylsulfonyl)phenyl]-4-oxo-3-phenyl-2-buten-1-yl ester (CA INDEX NAME)

RN 754242-09-6 ZCAPLUS

CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (22)-2-[4-(methylsulfonyl)phenyl]-4-[6-(nitrooxy)hexyl]oxy]-4-oxo-3phenyl-2-buten-1-yl ester (CA INDEX NAME)

Double bond geometry as shown.

RN 754242-12-1 ZCAPLUS

CN Benzeneacetic acid, α =[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, (α Z)-(CA INDEX NAME)

Double bond geometry as shown.

21

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L9 ANSWER 9 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:
                        2004:101124 ZCAPLUS
DOCUMENT NUMBER:
                         140:163574
TITLE:
                        Preparation of nitric oxide
                        releasing diary1-2-(5H)-furanone prodrugs as selective
                         cyclooxygenase-2 inhibitors for treatment inflammatory
                         diseases
INVENTOR(S):
                         Berthelette, Carl; Lachance, Nicholas; Li, Lianhai;
                         Sturing, Claudio; Wang, Zhaovin; Young, Robert N.;
                         Dufresne, Claude
PATENT ASSIGNEE(S):
                         Merck Frosst Canada & Co., Can.
SOURCE:
                         PCT Int. Appl., 129 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:
                         Patent
LANGUAGE:
                         English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
                                           APPLICATION NO.
     PATENT NO.
                        KIND DATE
                                                                  DATE
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                                           -----
                               20040205 WO 2003-CA1115
     WO 2004011421
                        A1
                                                                  20030724
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
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             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG,
             PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR,
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         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2493082
                              20040205 CA 2003-2493082
                         A1
                                                                 20030724
     AU 2003252515
                               20040216
                                         AU 2003-252515
                          A1
                                                                  20030724
     EP 1527045
                         A1
                               20050504
                                          EP 2003-771010
                                                                  20030724
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     US 20050261245
                         A1 20051124
                                            US 2005-521075
                                                                   20050112
     US 7199154
                         B2
                               20070403
PRIORITY APPLN. INFO.:
                                            US 2002-398683P
                                                              P 20020726
                                            US 2002-435341P
                                                              P 20021220
                                            WO 2003-CA1115
                                                              W 20030724
OTHER SOURCE(S):
                        CASREACT 140:163574; MARPAT 140:163574
IT
    654069-14-4P
     RL: BYP (Byproduct); PREP (Preparation)
        (preparation of nitric oxide releasing diarylfuranone
        prodrugs as selective cyclooxygenase-2 inhibitors for treatment of
        inflammatory diseases)
RN
    654069-14-4 ZCAPLUS
```

NAME)

Benzeneacetic acid, α -[2-[[3-[[[(1,1-

dimethylethyl)dimethylsilyl]oxy]methyl]benzoyl]oxy]-1-[4(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (aE)- (CA INDEX

IT 654068-75-4P 654068-76-5P 654068-79-8P 654068-81-2P 654068-81-2P 654068-81-2P 654068-81-2P 654068-81-2P 654068-87-8P 654068-89-P 654068-99-09 654068-99-09 F654068-99-09 F654068-99-09 F654068-99-09 F654068-90-09 F654068-90-0

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitric oxide releasing diarylfuranone prodrugs as selective cyclooxygenase-2 inhibitors for treatment of inflammatory diseases)

RN 654068-75-4 ZCAPLUS

CN Benzeneacstic acid, $\alpha = \{1 - [4 - (methylsulfonyl)phenyl] - 2 - [3 - (nitrooxy)methyl]benzoyl]oxy]ethylidene]-, methyl ester, <math>(\alpha Z) - (CA \times MAME)$

Double bond geometry as shown.

RN 654068-76-5 ZCAPLUS

CN Benzeneacetic acid, $\alpha=\{1-\{4-(methylsulfonyl)phenyl\}-2-[\{4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, methyl ester, (<math>\alpha$ Z)- (CA INDEX NAME)

- RN 654068-79-8 ZCAPLUS
- CN Benzeneacetic acid, $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, methyl ester, (<math>\alpha Z$)- (CA INDEX NAME)

- RN 654068-81-2 ZCAPLUS
- CN Benzeneacetic acid, α =[1-[4-(methylsulfonyl)phenyl]-2-[[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, ethyl ester, (α Z)- (CA INDEX NAME)

- RN 654068-83-4 ZCAPLUS
- CN Benzeneacetic acid, $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, (<math>\alpha$ Z)-

(CA INDEX NAME)

Double bond geometry as shown.

RN 654068-84-5 ZCAPLUS

CN Benzeneacetic acid, α =[1-[4-(methylsulfonyl)phenyl]-2-[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, ethyl ester, (α Z)-(CA INDEX NAME)

Double bond geometry as shown.

RN 654068-85-6 ZCAPLUS

CN Benzeneacetic acid, a-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, 2-(diethylamino)ethyl ester, (aZ)- (CA INDEX NAME)

- RN 654068-86-7 ZCAPLUS
- CN Benzeneacetic acid, a-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-2-(1,1-dimethylethoxy)-1-methyl-2-oxoethyl ester, (aZ)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

- RN 654068-87-8 ZCAPLUS
- CN Benzeneacetic acid, a-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-1-carboxyethyl ester, (aZ)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

- RN 654068-88-9 ZCAPLUS
- CN Benzeneacetic acid, a-[1-[4-(methylsulfonyl)phenyl]-2-[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, (α Z)-(CA INDEX NAME)

RN 654068-89-0 ZCAPLUS

CN Benzeneacetic acid, a=[1-[4-(methylsulfonyl)phenyl]-2-[[[5-(nitrooxy)pentyl)oxy]carbonyl]oxplethylidene]-, 2-(diethylamino)ethyl ester, hydrochloride (1:1), (a2)- (CA INDEX NAME)

Double bond geometry as shown.

HC1

RN 654068-90-3 ZCAPLUS

CN Benzeneacetic acid, a-[1-[4-(methylaulfonyl)phenyl]-2-[[[3-[(nitrooxy)methyl]phenoxy]carbonyl]oxy]ethylidene]-, methyl ester, (aZ)- (CA INDEX NAME)

- IT 654068-91-4P 654068-95-8P 654068-98-1P
 654069-03-1P 654069-03-P 654069-10-0P
 654069-11-1P 654069-15-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of nitric oxide releasing diarylfuranone
 prodrugs as selective cyclooxygenase-2 inhibitors for treatment of
 inflammatory diseases)
 RN 654068-91-4 ZCAPLUS
- CN Benzeneacetic acid, $\alpha = [2 [[3 [[(1, 1 dimethylethyl)dimethylsilylloxylmethyl]ben$

dimethylethyl)dimethylsilyl]oxy]methyl]benzoyl]oxy]-1-[4- (methylsulfonyl)phenyl]ethylidene]-, methyl ester, (α Z)- (CA INDEX NAME)

Double bond geometry as shown.

- RN 654068-95-8 ZCAPLUS
- CN Benzeneacetic acid, α =[2-[{(4-bromobutoxy)carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (α Z)- (CA INDEX NAME)

RN 654068-98-1 ZCAPLUS

CN Benzeneacetic acid, α-[2-[[(4-bromobutoxy)carbony1]oxy]-1-[4-(methylsulfony1)pheny1]ethylidene]-, ethyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

RN 654069-03-1 ZCAPLUS

CN Benzeneacetic acid, $\alpha-[2-[[[(6-bromohexyl)oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, <math>(\alpha Z)-$ (CA INDEX NAME)

Double bond geometry as shown.

RN 654069-09-7 ZCAPLUS

CN Benzeneacetic acid, $\alpha = [2 - [[[3 - [[[(1, 1 -$

 $\label{limits} $$ \dim thylsilyl[oxy] = honoxy[carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, $(\alpha Z)-$ (CA INDEX NAME)$ $$$

Double bond geometry as shown.

- RN 654069-10-0 ZCAPLUS
- CN Benzeneacetic acid, α -[2-[[[3-(hydroxymethyl)phenoxy]carbonyl]oxy]-1[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (α Z)- (CA
 INDEX NAME)

Double bond geometry as shown.

- RN 654069-11-1 ZCAPLUS
- CN Benzeneacetic acid, α -[2-[[[3-(bromomethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (α Z)- (CA INDEX NAME)

RN 654069-15-5 ZCAPLUS

CN Benzeneacetic acid, α -[2-[[3-(bromomethyl)benzoyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (\alpha Z)- (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 10 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 2001:472491 ZCAPLUS

DOCUMENT NUMBER: 135:76524

TITLE: Preparation of nitrosated and nitrosvlated cyclooxygenase-2 inhibitors

INVENTOR(S): Bandarage, Ramani R.; Bandarage, Upul K.; Fang,

Xinqin; Garvey, David S.; Letts, L. Gordon; Schroeder,

Joseph D.; Tam, Sang William Nitromed, Inc., USA PCT Int. Appl., 230 pp.

PATENT ASSIGNEE(S): SOURCE:

CODEN: PIXXD2 DOCUMENT TYPE:

Patent English

LANGUAGE: FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATE	KIN	D	DATE			APPL	ICAT	DATE									
WO 2001045703					A1 20010628			0628		WO 2	000-	20001222					
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    CA 2393724
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                              20040621
                                        MX 2002-6312
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                                         US 2003-463671
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PRIORITY APPLN. INFO.:
                                          US 1999-171623P
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                                          US 2006-599519
                                                            A3 20061115
                       MARPAT 135:76524
    346683-81-6P 346683-83-8P
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OTHER SOURCE(S):

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitrosated and nitrosylated

cyclooxygenase-2 inhibitors)

RN 346683-81-6 ZCAPLUS

CN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, 3-[4-[1-methvl-1-(nitrosothio)ethvl]-2-oxo-3-oxazolidinvl]propvl ester, (αZ)- (CA INDEX NAME)

RN 346683-83-8 ZCAPLUS

CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, 2-[1-methyl-4-(nitrosothio)-4-piperidinyl]ethyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT:

4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 11 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:462317 ZCAPLUS

DOCUMENT NUMBER: 125:114294

ORIGINAL REFERENCE NO.: 125:21435a,21438a

TITLE: Preparation of stilbene derivatives useful as

cyclooxygenase-2 inhibitors

INVENTOR(S): Atkinson, Joseph G.; Wang, Zhaoyin PATENT ASSIGNEE(S): Merck Frosst Canada Inc., Can.

SOURCE: PCT Int. Appl., 80 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

							DATE	APPLICATION NO.							DATE				
	WO 9613483								WO 1995-CA601						19951024				
	₩:						BR,												
							LT,						MN,	MX,	NO,	NZ,	PL,	RO,	
	RW:						UG,						DK.	ES.	FR.	GB.	GR.	IE.	
							SE,												
		NE,	SN,	TD,	TG														
CA	2200462				A1 19960509				CA 1995-2200462						19951024				
AU	AU 9536950			A 19960523			AU 1995-36950						19951024						
AU	6889	80			B2		1998	0319											
EP	7884	76			A1		1997	0813		EP	19	95-	9447	87			19951	024	
EP	7884	76			В1		1999	1020											
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AT	1857	97			T		1999	1115		ΑT	19	95-	9447	87		:	19951	024	
ES	2139	959			Т3		2000	0216		ES	19	95-	9447	87			19951	024	
US	5849	943			A		1998	1215		US	19	97-	8171:	28			19970	407	
PRIORIT						US	19	94-	3301	72		A1 :	19941	027					
										WO	19	95-0	CA60	1		W :	19951	024	
OTHER S	OTHER SOURCE(S):						125:												

ΙT 179174-84-6P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of stilbene derivs. useful as cyclooxygenase-2 inhibitors) RN 179174-84-6 ZCAPLUS

Benzeneacetic acid, $\alpha - (2 - (acetvloxv) - 1 - (4 -$

(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

- 179174-89-1 179174-90-4 179174-95-9 179175-00-9 179175-04-3 179175-09-8
 - 179175-14-5

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of stilbene derivs. useful as cyclooxygenase-2 inhibitors)

RN 179174-89-1 ZCAPLUS

Benzeneacetic acid, α -[2-(benzoyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

RN 179174-90-4 ZCAPLUS

CN Benzeneacetic acid, a-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 179174-95-9 ZCAPLUS CN Benzeneacetic acid,

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 179175-00-9 ZCAPLUS

CN Benzeneacetic acid, $\alpha - \{2 - (acetyloxy) - 1 - \{4 - (aminosulfonyl)phenyl\}ethylidene] -, methyl ester, (Z) - (9CI) (CA INDEX NAME)$

RN 179175-04-3 ZCAPLUS CN Benzeneacetic acid, a-[1-[4-(aminosulfonyl)phenyl]-2-(benzoyloxy)ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 179175-09-8 ZCAPLUS CN Benzeneacetic acid, α

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 179175-14-5 ZCAPLUS

CN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 10:54:15 ON 17 JUN 2009)

FILE 'REGISTRY' ENTERED AT 10:54:48 ON 17 JUN 2009

STRUCTURE UPLOADED

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FILE 'ZCAPLUS' ENTERED AT 11:14:23 ON 17 JUN 2009 E US2006-586573/APPS

1 S US2006-586573/APPS

L4

SEL RN

FILE 'REGISTRY' ENTERED AT 11:15:49 ON 17 JUN 2009

34 S E1-E34

4 S L3 AND L5 L6

FILE 'ZCAPLUS' ENTERED AT 11:18:58 ON 17 JUN 2009

L7 18 S L3

L8 1 S L7 AND (NITROSATED OR NITROSYLATED)

L9 11 S L7 AND (NITROSATED OR NITROSYLATED OR NO OR (NITRIC (W) OXIDE

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LOGOFF? (Y)/N/HOLD:v

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 67.29 277.05

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